

On the implicit restart of the rational Krylov method

Chasing algorithms for polynomial, extended and rational Krylov

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Problem statement

Single sentence problem statement

We want to compute a small number of eigenpairs of $A \in \mathbb{C}^{N \times N}$ that satisfy some property \mathfrak{P} .

Examples:

- All eigenvalues in a domain $\Omega \subset \mathbb{C}$
- The eigenvalue(s) with largest real part
- The eigenvalue(s) closest to the imaginary axis

Polynomial Krylov

Polynomial Krylov

Definition (Krylov subspace)

Given a matrix $A \in \mathbb{C}^{N \times N}$ and a vector $\mathbf{0} \neq \mathbf{v} \in \mathbb{C}^N$:

$$\mathcal{K}_{m+1} = \mathcal{K}_{m+1}(A, \mathbf{v}) := \text{span}\{\mathbf{v}, A\mathbf{v}, \dots, A^m\mathbf{v}\}.$$

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- Assumption: subspace is A -variant: $A\mathcal{K}_{m+1} \not\subseteq \mathcal{K}_{m+1}$.
- Isomorphism: $\mathcal{K}_{m+1} \cong \mathcal{P}_m$, i.e. $\forall \mathbf{w} \in \mathcal{K}_{m+1}, \exists p \in \mathcal{P}_m : \mathbf{w} = p(A)\mathbf{v}$ and vice versa.
- Orthogonal basis $V \in \mathbb{C}^{N \times (m+1)}$ such that

$$\text{span}\{V_{(:,1:k+1)}\} = \text{span}\{\mathbf{v}, A\mathbf{v}, \dots, A^k\mathbf{v}\} \quad \forall k \leq m.$$

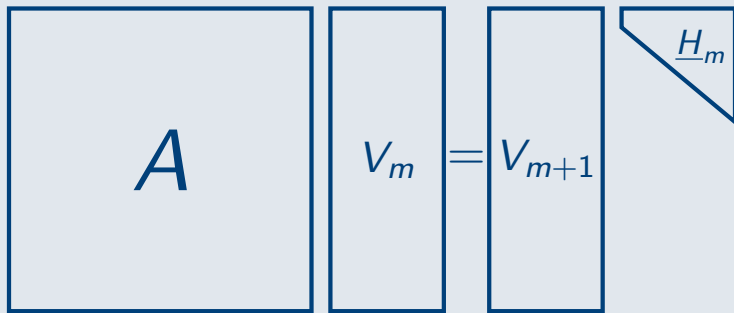
Arnoldi's method: recurrence relation

$$A V_m = V_m H_m + h_{m+1,m} v_{m+1} e_m^T$$

Arnoldi's method: recurrence relation

$$A V_m = V_{m+1} \underline{H}_m$$

Arnoldi's method: recurrence relation



The diagram illustrates the recurrence relation for Arnoldi's method. It consists of a large square box labeled A on the left. To its right is a vertical rectangular box labeled V_m . An equals sign is placed between V_m and another vertical rectangular box labeled V_{m+1} . To the right of V_{m+1} is a right-angled triangle. The hypotenuse of the triangle is a diagonal line from the top-left corner to the bottom-right corner. The label \underline{H}_m is positioned in the upper-left area of the triangle, representing the m -th Hessenberg matrix.

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\Rightarrow Compute the **Ritz pairs**

Small scale eigenvalue problem:

$$H_m \mathbf{z} = \vartheta \mathbf{z}$$

Ritz pairs $(\vartheta, \mathbf{x}) := (\vartheta, V_m \mathbf{z})$ satisfy Galerkin condition $A \mathbf{x} - \vartheta \mathbf{x} \perp \mathcal{K}_m$

What if the eigenvalues of A that satisfy \mathfrak{P} only converge for $m \rightarrow N$?

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- **Explicit restart:** for certain maximal m , select $\mathbf{w} \in \mathcal{K}_{m+1}$ and continue constructing new $\mathcal{K}_{m+1}(A, \mathbf{w})$ from scratch (Saad, 1980).
- **Implicit restart:** for certain maximal m , apply l -th order *polynomial filter* and continue from k -th order $\mathcal{K}_{k+1}(A, \hat{\mathbf{v}})$ ($l + k = m$) (Sorensen, 1992).
- **Krylov-Schur:** compute and reorder the Schur decomposition of H_m (Stewart, 2001).

Implicitly restarted Arnoldi (IRA)

Input: $(V_{m+1}, \underline{H}_m), \{\varrho_i\}_{i=1}^l$

1: **for** $i = 1 \dots l$ **do**

$$2: \quad \underline{H}_{m-i+1} - \varrho_i \underline{L}_{m-i+1} = \begin{bmatrix} Q & q \end{bmatrix} \begin{bmatrix} R \\ 0 \end{bmatrix}$$

$$3: \quad \underline{H}_{m-i} := Q^* \underline{H}_{m-i+1} Q_{(1:m-i+1, 1:m-i)}$$

$$4: \quad V_{m-i+1} := V_{m-i+2} Q$$

5: **end for**

$$6: \quad \textbf{return} \quad \hat{V}_{k+1} := V_{k+1}, \hat{H}_k := \underline{H}_k$$

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- 4: $V_{m-i+1} := V_{m-i+2} Q$
- 5: **end for**
- 6: **return** $\hat{V}_{k+1} := V_{k+1}, \hat{H}_k := \underline{H}_k$

Result: $\hat{V}_{k+1} \mathbf{e}_1 = \prod_{i=1}^l (A - \varrho_i I) \mathbf{v}$

Practical implementation: Implicit-Q theorem

The Arnoldi decomposition $(V_{m+1}, \underline{H}_m)$ of order m is uniquely¹ defined by the matrix A and first column $V\mathbf{e}_1$.

¹*essential uniqueness*

Polynomial Krylov

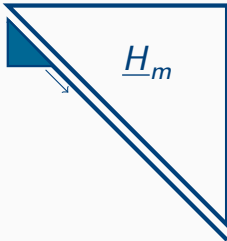
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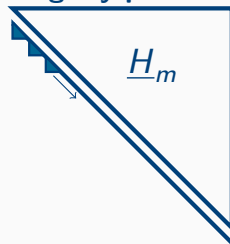
Single



Multi



Tightly-packed



¹essential uniqueness

Illustrative example

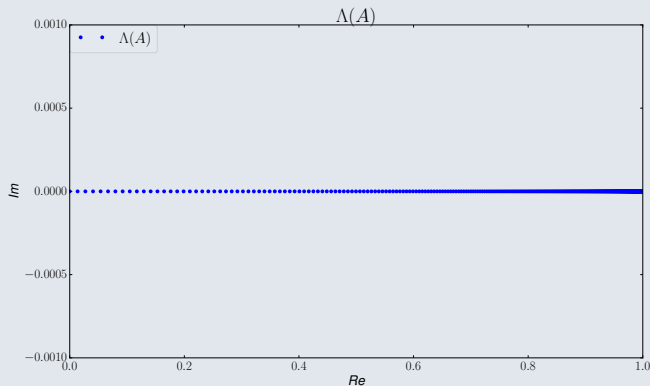
$A \in \mathbb{R}^{500 \times 500}$, $\Lambda(A) \subset [0, 1]$, \mathfrak{P} : rightmost eigenvalue

Diagonal matrix, logarithmically spaced eigenvalues

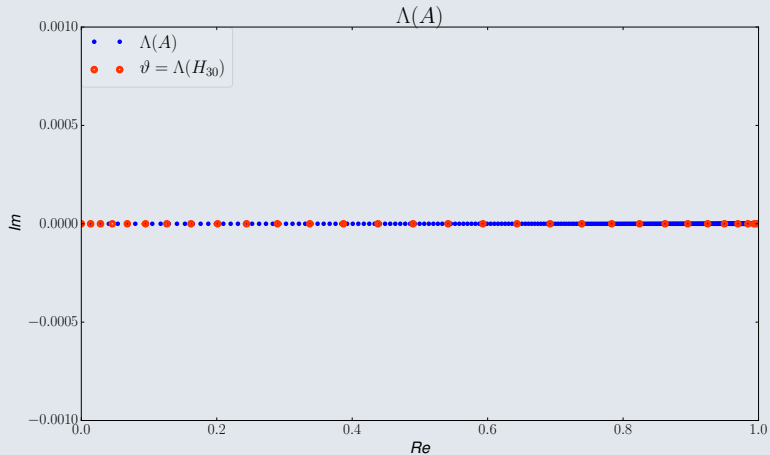
Illustrative example

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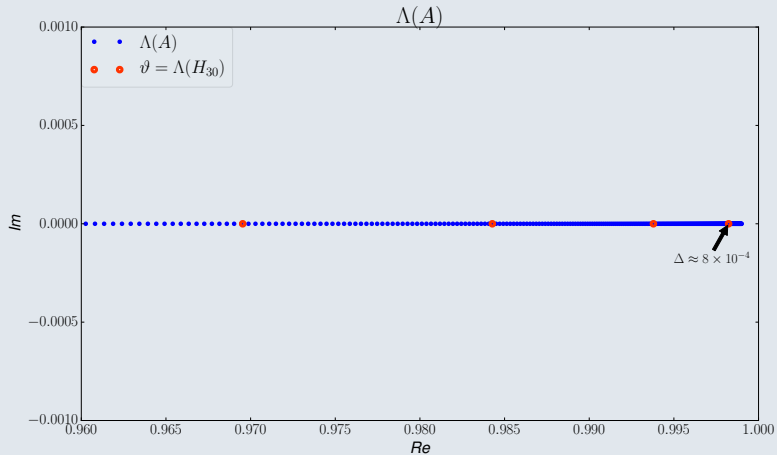
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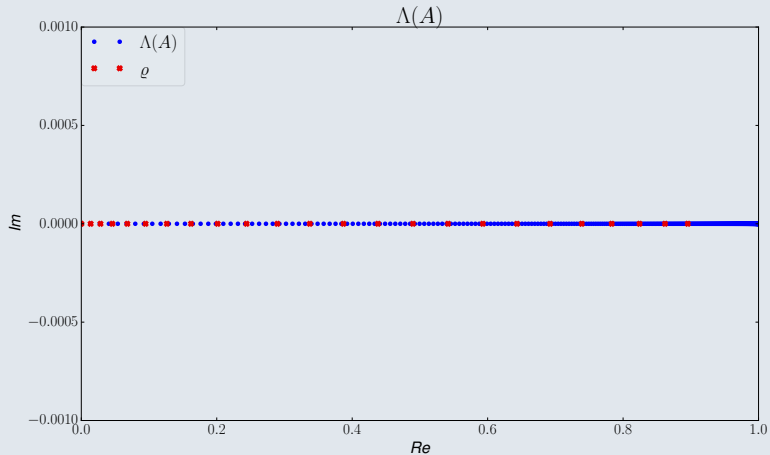
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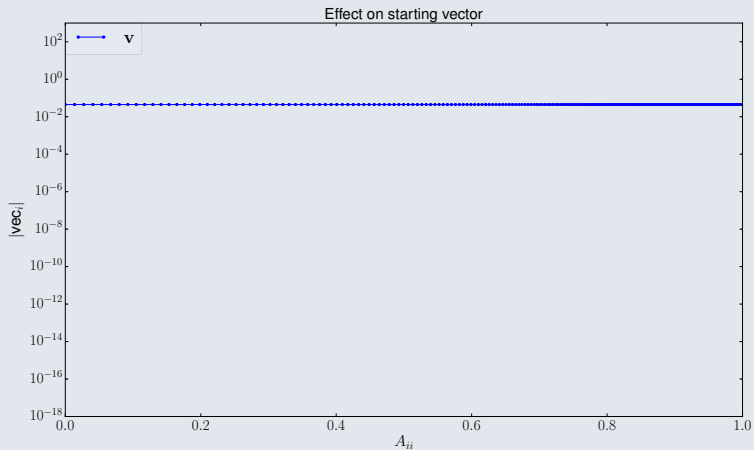
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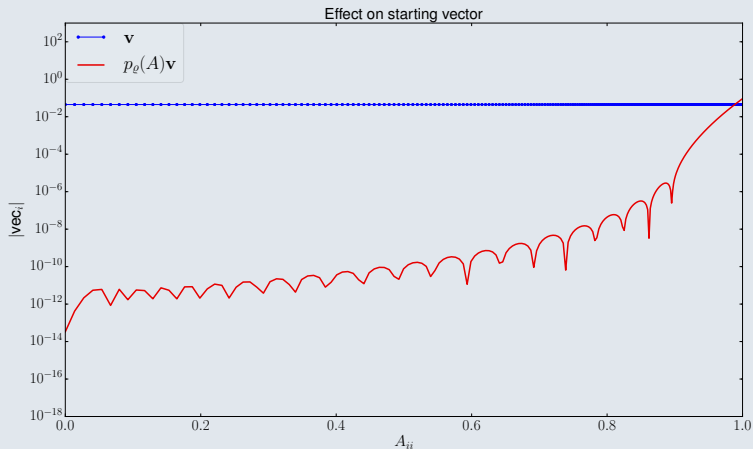
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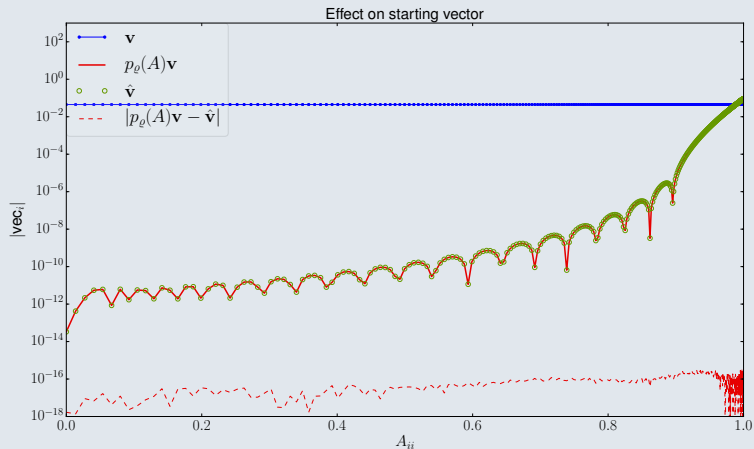


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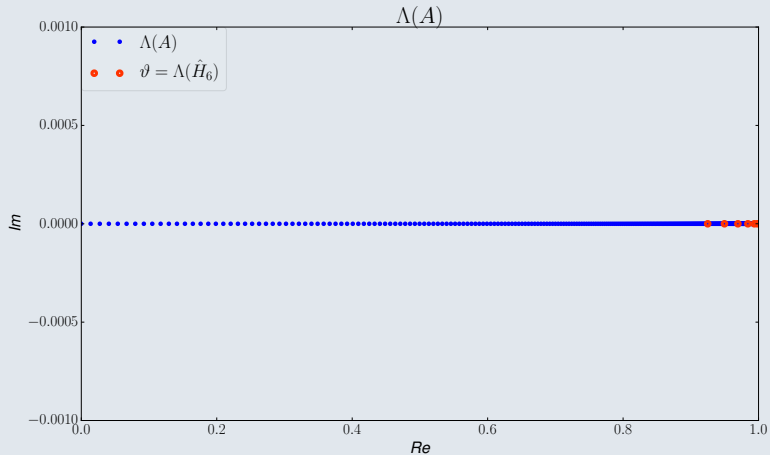


Polynomial Krylov

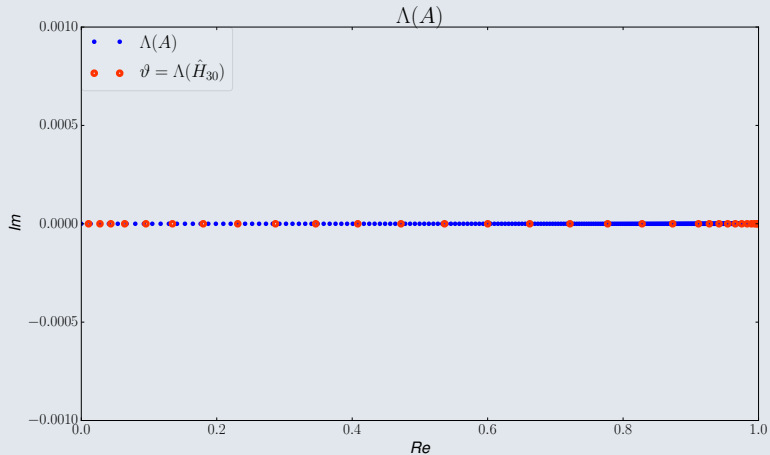
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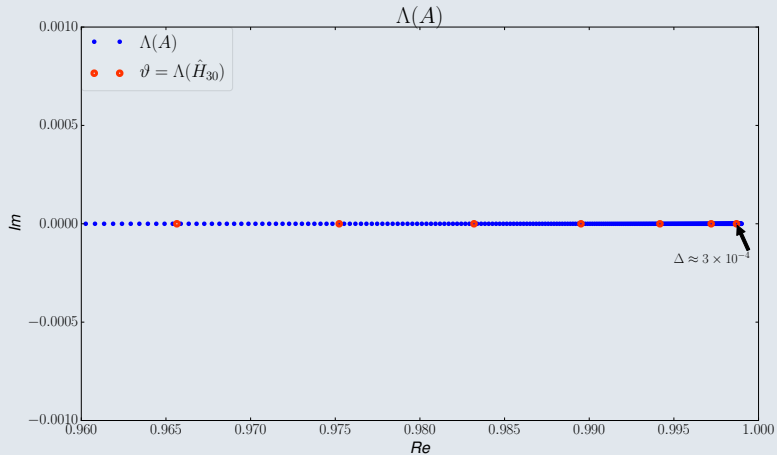


Illustrative example



Polynomial Krylov

Illustrative example



Rational Krylov

Definition (Rational Krylov sequence (Berljafa and Güttel, 2015))

Given a matrix $A \in \mathbb{C}^{N \times N}$, a vector $\mathbf{0} \neq \mathbf{v} \in \mathbb{C}^N$ and $q_m \in \mathcal{P}_m$ with roots $\Xi = \{\xi_1, \dots, \xi_m\} \in \overline{\mathbb{C}} \setminus \Lambda(A)$:

$$\mathcal{Q}_{m+1}(A, \mathbf{v}, \Xi) = \mathcal{Q}_{m+1}(A, \mathbf{v}, q_m) := q_m(A)^{-1} \mathcal{K}_{m+1}(A, \mathbf{v}).$$

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Isomorphism: $\mathcal{Q}_{m+1} \cong q_m(z)^{-1} \mathcal{P}_m$, i.e. $\forall \mathbf{w} \in \mathcal{Q}_{m+1}, \exists p \in \mathcal{P}_m : \mathbf{w} = q_m(A)^{-1} p(A) \mathbf{v}$

Rational Arnoldi's method (Ruhe, 1998): recurrence relation

$$A V_{m+1} \underline{K}_m = V_{m+1} \underline{L}_m$$

Rational Arnoldi's method (Ruhe, 1998): recurrence relation

The diagram illustrates the recurrence relation for Rational Arnoldi's method. It shows a large square matrix A multiplied by a tall rectangular vector V_{m+1} . This product is then multiplied by a triangular matrix \underline{K}_m , which has a diagonal line from the top-left to the bottom-right. This entire expression is set equal to another tall rectangular vector V_{m+1} multiplied by a triangular matrix \underline{L}_m , which also has a diagonal line from the top-left to the bottom-right.

$$A V_{m+1} \underline{K}_m = V_{m+1} \underline{L}_m$$

Rational Krylov

Rational Arnoldi's method (Ruhe, 1998): recurrence relation

$$\begin{bmatrix} A \end{bmatrix} \begin{bmatrix} V_{m+1} \end{bmatrix} \begin{bmatrix} \xi_1 & & & \\ & \xi_2 & & \\ & & \ddots & \\ & & & \xi_m \end{bmatrix} \begin{bmatrix} K_m \end{bmatrix} = \begin{bmatrix} V_{m+1} \end{bmatrix} \begin{bmatrix} \xi_1 & & & \\ & \xi_2 & & \\ & & \ddots & \\ & & & \xi_m \end{bmatrix} \begin{bmatrix} L_m \end{bmatrix}$$

Rational Arnoldi's method (Ruhe, 1998): recurrence relation

$$\begin{array}{|c|} \hline A \\ \hline \end{array} \begin{array}{|c|} \hline V_{m+1} \\ \hline \end{array} \begin{array}{|c|} \hline \begin{array}{c} \xi_1 \quad \quad \quad \underline{K}_m \\ \xi_2 \quad \quad \quad \diagdown \\ \vdots \quad \quad \quad \vdots \\ \xi_m \end{array} \\ \hline \end{array} = \begin{array}{|c|} \hline V_{m+1} \\ \hline \end{array} \begin{array}{|c|} \hline \begin{array}{c} \xi_1 \quad \quad \quad \underline{L}_m \\ \xi_2 \quad \quad \quad \diagdown \\ \vdots \quad \quad \quad \vdots \\ \xi_m \end{array} \\ \hline \end{array}$$

*(Abuse of) notation: $l_{i+1,i}/k_{i+1,i} = \xi_i$

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Ritz pairs $(\vartheta, \mathbf{x}) := (\vartheta, V_{m+1} \underline{K}_m \mathbf{z})$ satisfy Galerkin condition

$$A \mathbf{x} - \vartheta \mathbf{x} \perp \mathcal{K}_m(A, q_m(A)^{-1} \mathbf{v})$$

What if the eigenvalues of A that satisfy \mathfrak{P} only converge for $m \rightarrow N$?

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Same solutions as before!

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- **Implicit restart:** for certain maximal m , apply l -th order *polynomial filter* and continue from k -th order $\mathcal{Q}_{k+1}(A, \hat{\mathbf{v}}, q_k)$ ($l + k = m$) (De Samblanx et al., 1997).
- **Krylov-Schur:** compute and reorder the generalized Schur decomposition of (L_m, K_m) (De Samblanx et al., 1997).

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Special case: extended Krylov introduced by Druskin and Knizhnerman (1998)

$$\Xi_{\text{ext}} = \{\xi_i\}_{i=1}^m, \forall i : \xi_i \in \{0, \infty\}$$

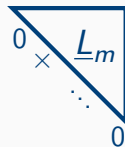
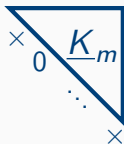
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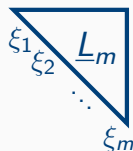
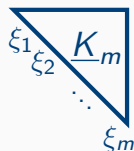
Example: $\Xi_{\text{ext}} = \{0, \infty, \dots, 0\}$



The matrix pencil is in *condensed* format, chasing by elementary unitary operations (Camps et al., 2016)

How to apply the polynomial filter implicitly?

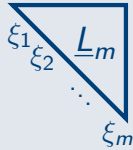
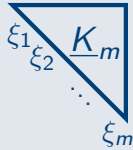
General case:



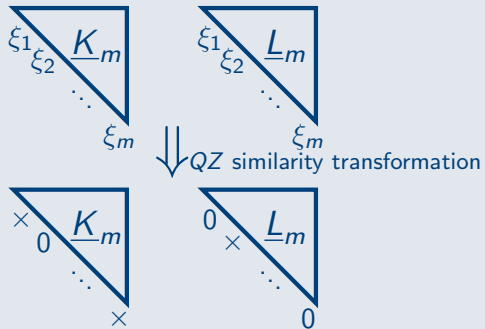
No longer in condensed format!

Rational Krylov

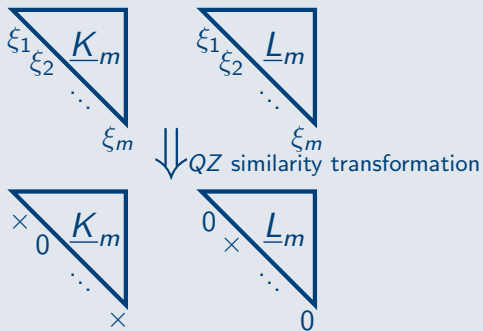
Solution



Solution

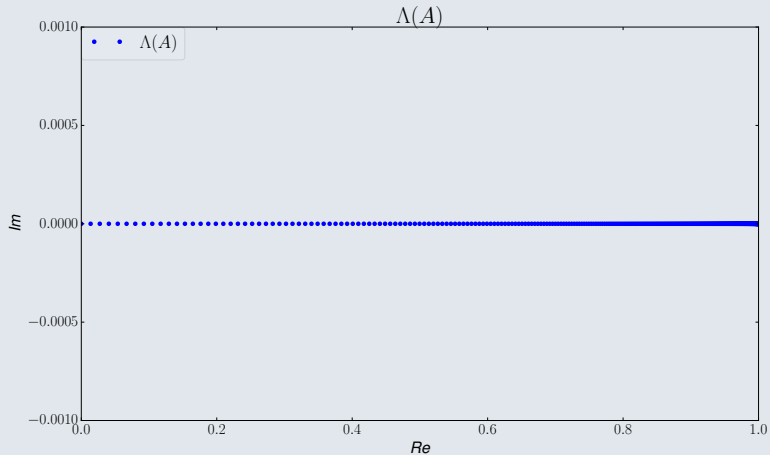


Solution

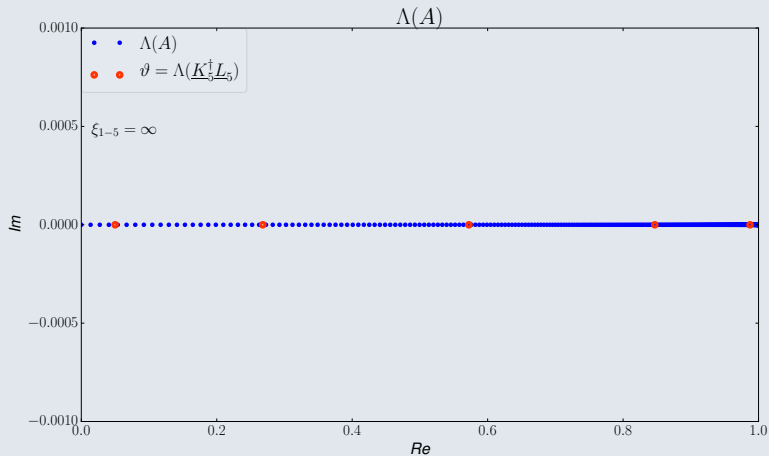


The QZ transformation is formulated in terms of elementary transformations on core transformations

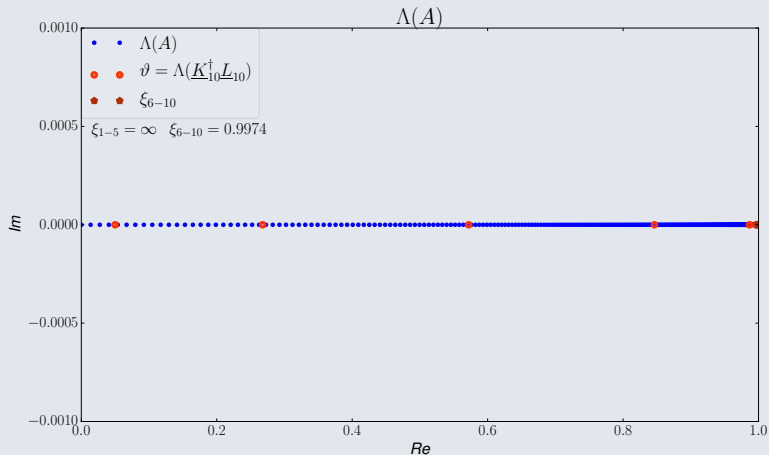
Illustrative example



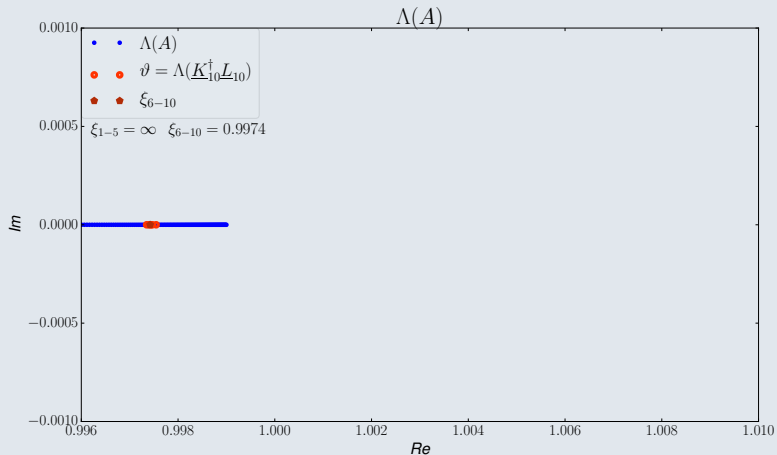
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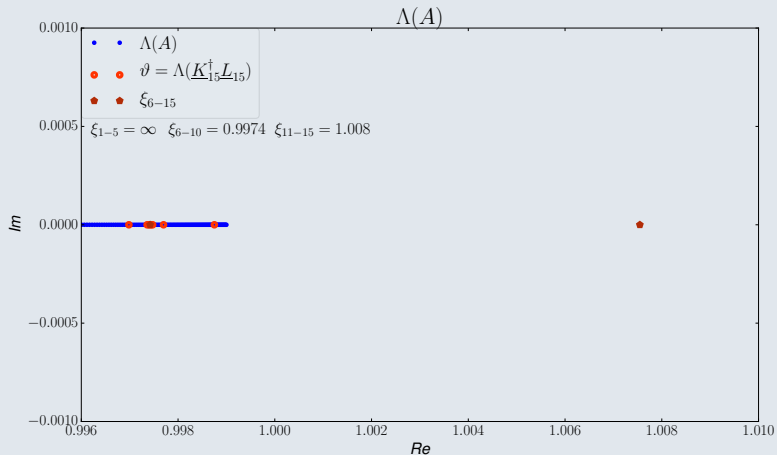
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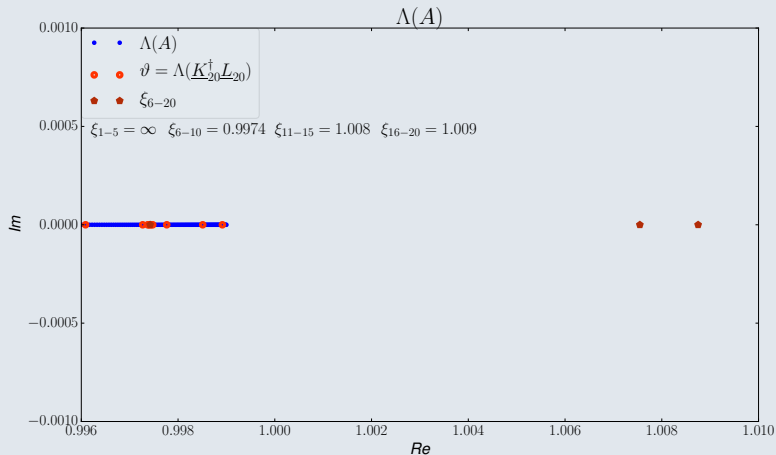
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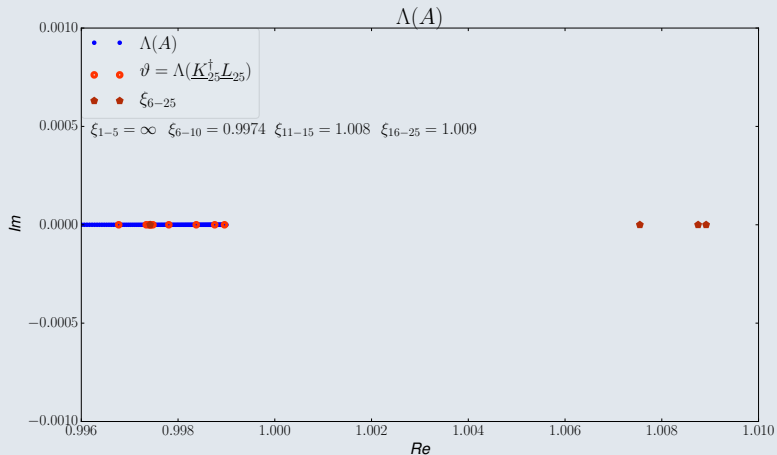
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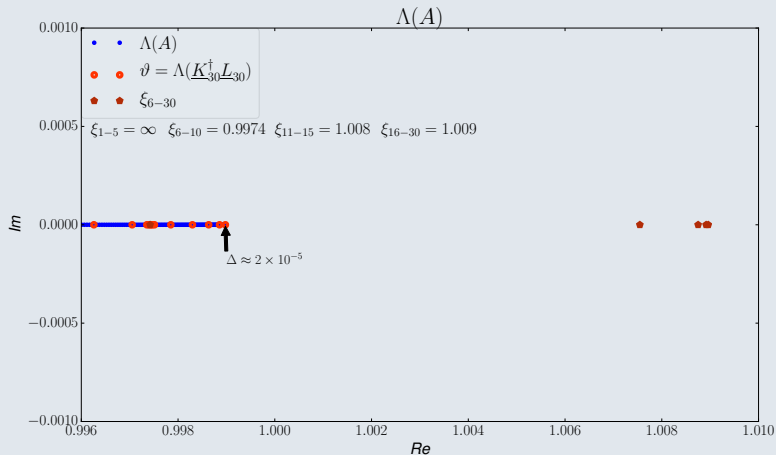
Illustrative example



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Illustrative example

Transformation: $(V_{m+1}, \underline{K}_m, \underline{L}_m) \rightarrow (\tilde{V}_{m+1}, \tilde{\underline{K}}_m, \tilde{\underline{L}}_m)$ with $\Xi_{\text{ext}} = \{\infty, 0, \infty, 0, \dots, 0\}$

Illustrative example

Transformation: $(V_{m+1}, \underline{K}_m, \underline{L}_m) \rightarrow (\tilde{V}_{m+1}, \tilde{\underline{K}}_m, \tilde{\underline{L}}_m)$ with $\Xi_{\text{ext}} = \{\infty, 0, \infty, 0, \dots, 0\}$

$$\mathcal{Q}_{m+1}(A, \mathbf{v}, q_m) = \tilde{\mathcal{Q}}_{m+1}(A, \mathbf{w}, \Xi_{\text{ext}}) \quad \Rightarrow \quad \mathbf{w} = \alpha q_m(A)^{-1} A^{m/2} \mathbf{v}$$

Illustrative example

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Ritz values are **not** affected: $\tilde{\underline{K}}_m = Q \underline{K}_m Z, \quad \tilde{\underline{L}}_m = Q \underline{L}_m Z$

Illustrative example

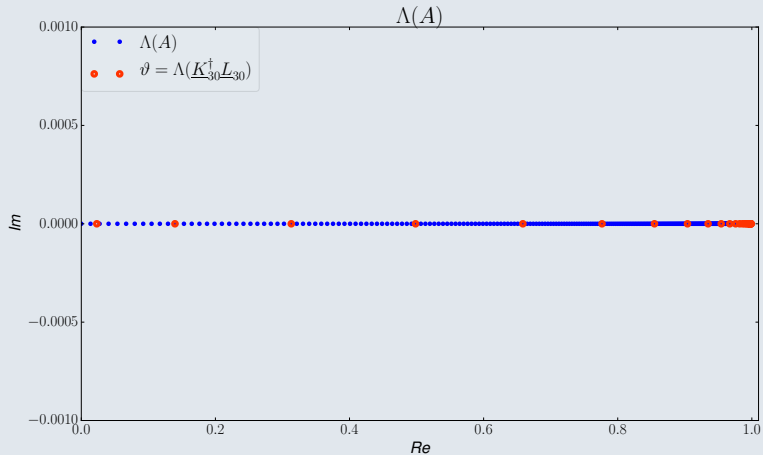
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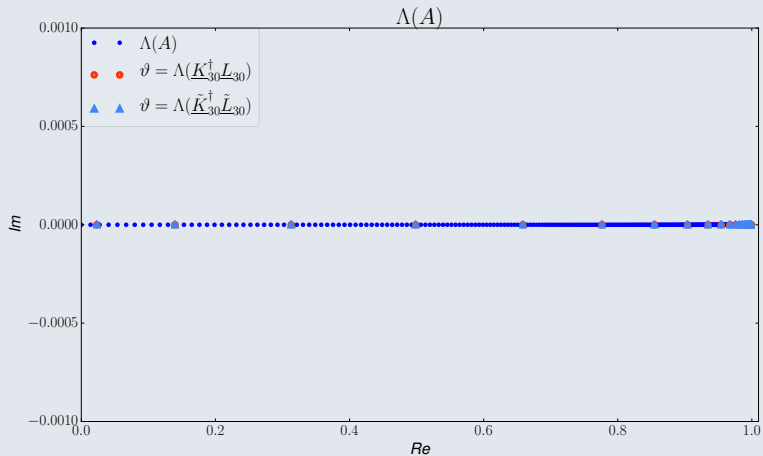
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$$\tilde{\underline{K}}_m^\dagger \tilde{\underline{L}}_m = Z^* \underline{K}_m^\dagger Q^* Q \underline{L}_m Z$$

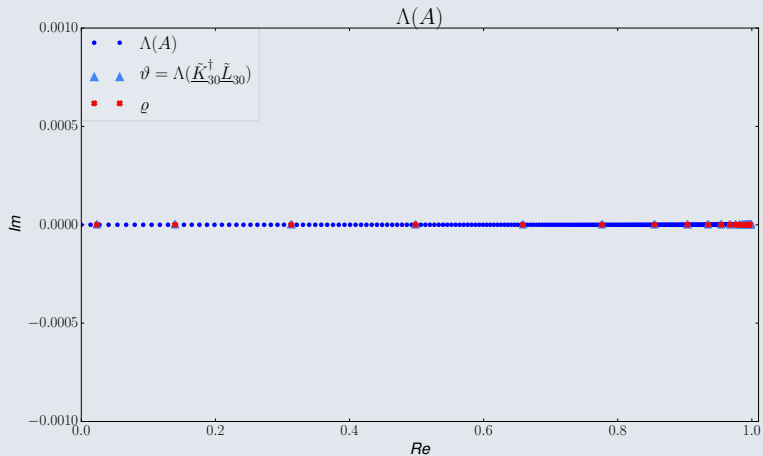
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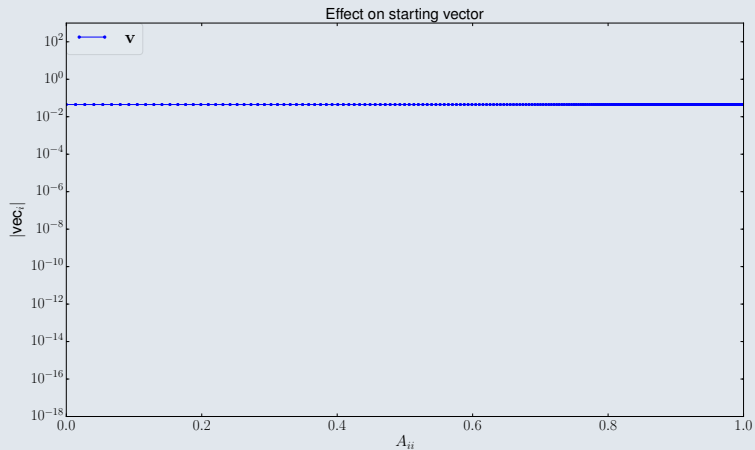
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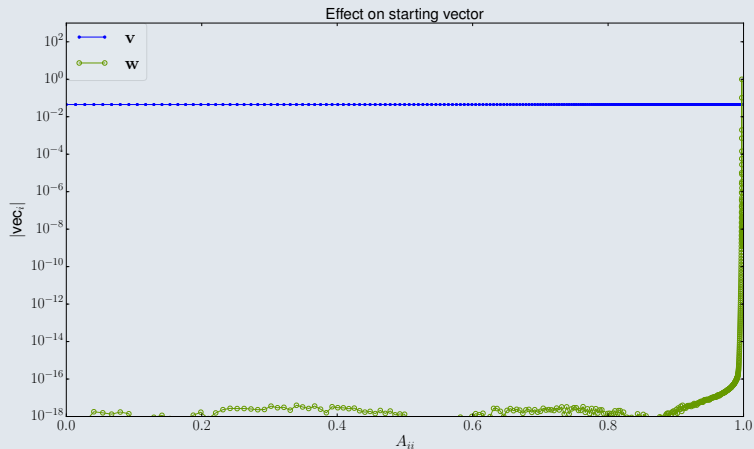
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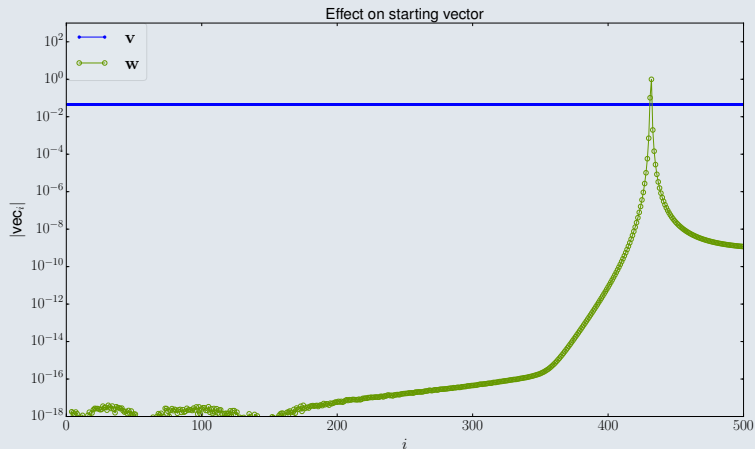
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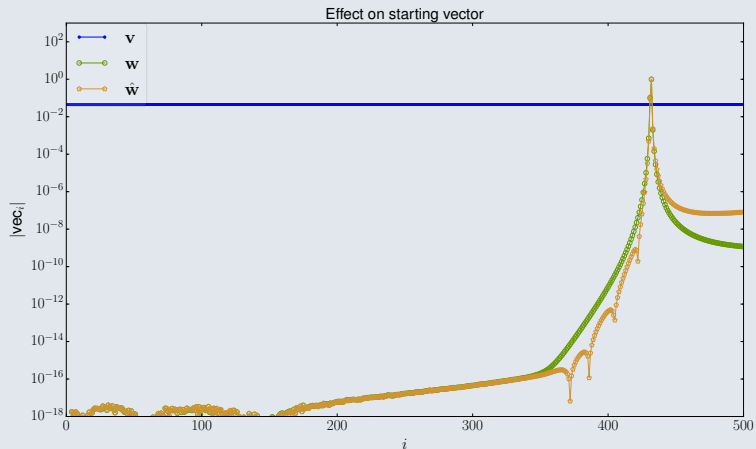
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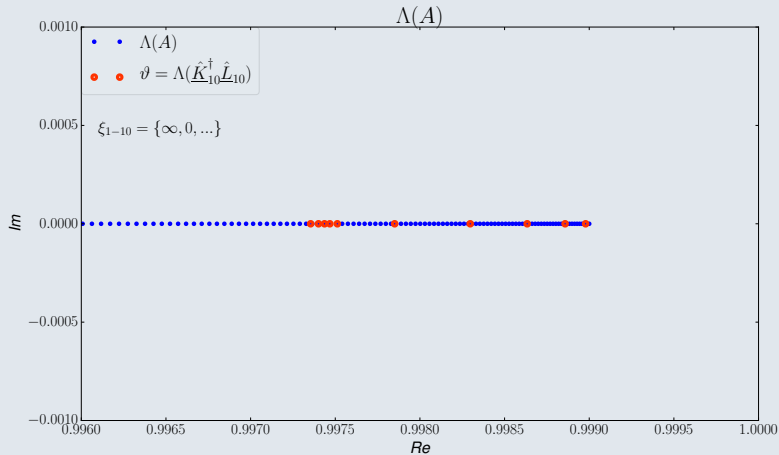
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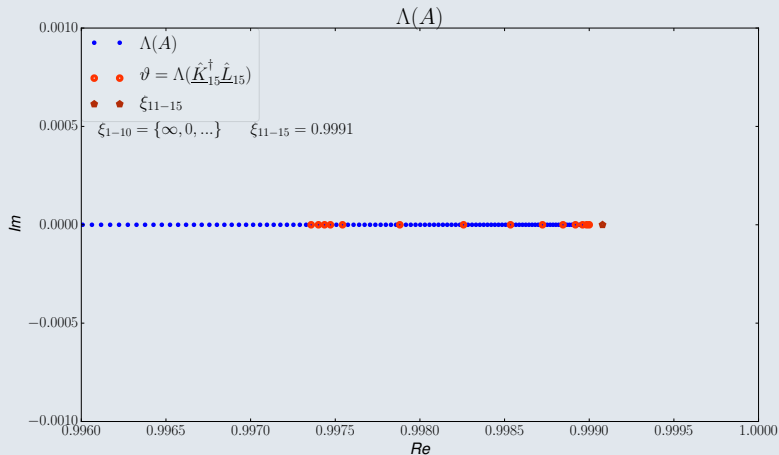
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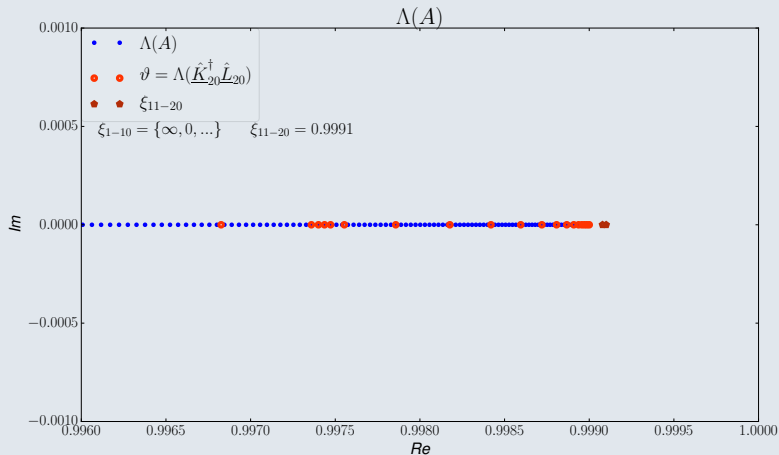
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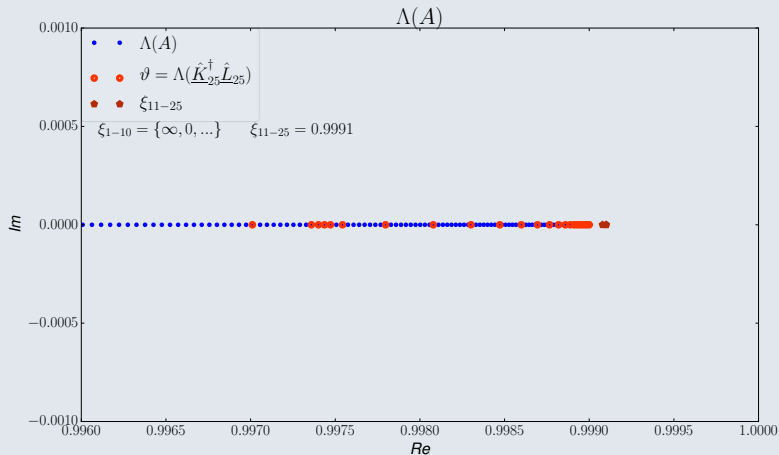
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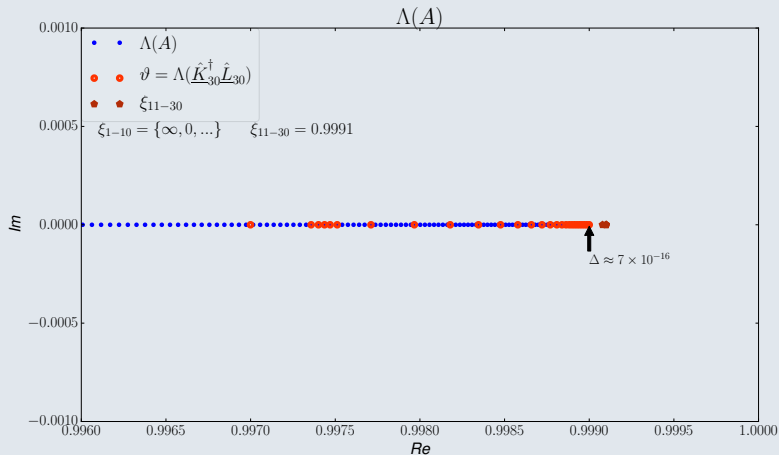
Illustrative example



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Illustrative example



Conclusion

- Filtering (rational) Krylov subspaces is useful to limit subspace dimension when searching for eigenvalues satisfying a property \mathfrak{P}
- The filter can be applied implicitly by means of elementary unitary operations (*chasing*) both for polynomial and rational Krylov

Thank you

References

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